Gaussian Background Model For the JBREWS Program

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Abstract: A computer model based on random superposition of upwind plumes is used to simulate the aerosol backgrounds expected in JBREWS scenarios. The user specifies the background count rate and the computes the mean number of sources and average source strength required to give this background. Random number generators are then used to generate a pseudo-random background meeting the user description. Particle binning by size is included. Up to 25 detectors operating simultaneously are included in the simulation.

INTRODUCTION

Background data exist for single detectors that have been used at various test sites, most notably Dugway Proving Grounds. For example, the ACTD web site[1] contains 24 data sets for six aerodynamic particle sizer (APS) detectors each that were conducted during November 1996. In these data sets there are 62 particle size bins. Counts are recorded every 10 seconds. However good this data may be, we do not have access to background data for arrays of detectors operated simultaneously or operated at places other than Dugway.

A need therefore exists for a simulation program that will predict the performance of an array of detectors under realistic background conditions. It is hoped that this code will be useful for predicting how arrays of “dry” detectors (such as APS or MET-1 counters) can be used in conjunction with “wet” detectors to form an optimal JBREWS system as tested against the various scenarios, with background included. An important part of this simulation will be the simulation of the background itself.

The model described here is based on the Gaussian plume model.[2] A random superposition of upwind plumes is used to simulate the background. The user specifies the background count rate in each particle size bin. The code computes the mean number of sources and average source strength required to give this background. Random number generators are then used to generate a pseudo-random background meeting the user description. Particle binning by size is included. The user specifies the ratios of the particle bin populations with respect to one another and the code on the average delivers that distribution. Random fluctuations in those ratios with time are included in the simulation.

COORDINATE SYSTEM

In order to derive the model equations, one imagines a point source of dust in air space, with no walls or other boundaries. The location of the source is (x',y',z') and the time of release is t'. There is a detector for dust particles located at (x,y,z) in this coordinate system. There is a wind drift that is only in the -x direction and only has one value, u. Dust particles that are emitted from a source instantly reach a drift speed that is equal to u in the x direction, and they also obtain a settling velocity in the z direction, given by v_z. The settling velocity is a function of particle size.[3]

In this coordinate system, the upwind direction is +x. The wind velocity $u < 0$ and the settling velocity $v_z < 0$. Source particles generally are released at x' values such that $x' > x$ in order to be measured by the detector. The detector is turned on at time $t = 0$, and therefore begins its measurement of particles that were released at times $t < 0$. Figure 1 shows a typical dust plume resulting from a release of 1 billion dust particles in this coordinate system.

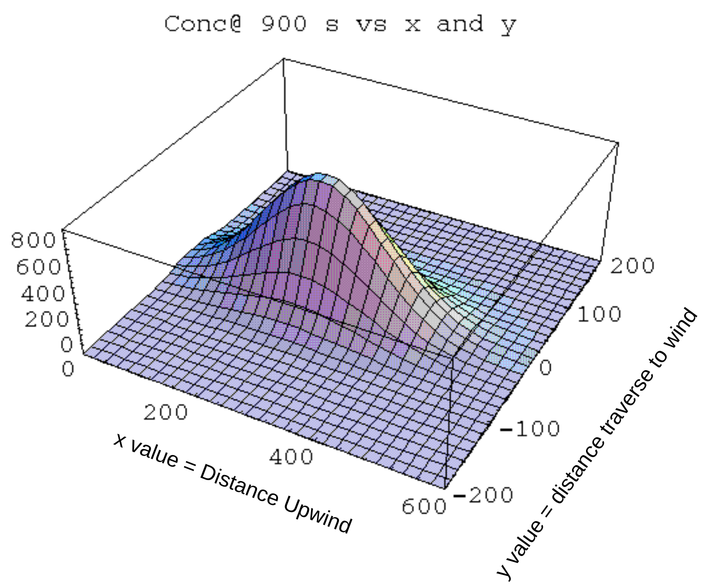

Figure 1. A Gaussian plume is shown for illustrative purposes, generated with Mathematica 2.0. Distances are in meters. Here, there is an instantaneous point release of a billion particles at the point x = 2500 m, y = 0 m at time t = 0. The drift velocity of the wind is 2.5 m/s in the negative x direction. The concentration is shown in units of particles/cubic meter.

GAUSSIAN PLUME MODEL ASSUMPTIONS

We assume no agglomeration or dissociation of particles from point of release until the moment of measure. Under these circumstances the concentration at the detector due to the source is governed by the continuity equation. Gaussian dispersion is assumed in vertical, longitudinal and transverse directions. Under these circumstances the measured concentration of the dust particles at the detector due to a unit release of dust is given by:

[1] $G_j(x,x',y,y',z,z',t-t')$

$$= \frac{e^{-[\{x - x' - u(t-t')\}/\sqrt{2}\,\sigma_x]^2}}{\sqrt{2\pi}\cdot\sigma_x} \cdot \frac{e^{-[\{y - y'\}/\sqrt{2}\,\sigma_y]^2}}{\sqrt{2\pi}\cdot\sigma_y} \cdot \frac{e^{-[\{z - z' - v_j(t-t')\}/\sqrt{2}\,\sigma_z]^2}}{\sqrt{2\pi}\cdot\sigma_z}$$

where

- G_j is concentration in mass or particles of size index j per cubic meter,
- x is downwind distance at which to evaluate the concentration in meters,
- y is lateral distance at which to evaluate the concentration in meters,
- z is height above ground at which to evaluate the concentration in meters,
- t is time of the measurement in seconds,
- x' is the upwind coordinate of the release in meters,
- y' is lateral coordinate of the release in meters,
- z' is height above ground of the release in meters,
- t' is time when the release occurred.
- σ_x is the dispersion coefficient in the direction of cloud travel in meters,
- σ_y is the dispersion coefficient in the transverse direction in meters,
- σ_z is the dispersion coefficient in the vertical direction in meters,
- u is the mean wind speed in meters per second (< 0),
- v_j is the mean settling velocity in meters per second (< 0) for this particle size.

We used the Pasquill-Gifford model[4] for the form of the dispersion coefficients, and chose values for constants in the expression from a National Oceanic and Atmospheric Administration (NOAA) report[5] for atmospheric stability class E, a condition that we judged to be conducive to effective agent dispersion. Thus, the dispersion coefficients are given by $\sigma_x = 52\left(x_d/\ 1000\right)^{0.88}$ and $\sigma_z = 23\left(x_d/\ 1000\right)^{0.51}$ with all quantities in meters as above. The quantity x_d is just the product $|u(t - t')|$. Other expressions for the dispersion coefficients could be used, for other conditions for example, and would work equally well.

The measured concentration due to all sources in a general case, under model assumptions, is then given by the integral over all source volume and all time of all point sources:

[2] $$c_j(x,y,z,t) = \int_{-\infty}^{t} \iiint_V S_j(x',y',z',t')\,G_j(x,x',y,y',z,z',t-t')\,dx'\,dy'\,dz'\,dt'$$

It is to be noted that the boundary conditions implied by the use of this Green's function ignore the influence of the ground on the concentration profile. At the ground, there could be reflection or clinging. In fact, there is a thin boundary layer of air near the ground where turbulence is not present and the basic motion equations are different than in the model. For this and many other reasons, it can be assured that the model will not be a very accurate predictor of dust settling behavior on surfaces. It is hoped that the overall atmospheric transport predictions are not greatly upset by these neglected boundary effects.

AVERAGE BEHAVIOR

One of the first questions that we want to answer is, how is the average behavior of the dust concentration determined? For instance, if we assume that there is a certain average concentration $\langle c_j \rangle$ of dust particles of size bin j, and a uniform source distribution upwind as an average, what value of S_j is required to give this average? In this case, we use the time-independent form of the Green's function. That is, the measured concentration at (x,y,z) due to a unit continuous source at (x′,y′,z′). The average measured concentration is then related to the average volumetric source density $\langle S_j \rangle$ through the equation:

$$[3] \qquad \langle c_j \rangle(x,y,z) = \iiint_V \langle S_j \rangle \; g_j(x,x',y,y',z,z')\, dx'\, dy'\, dz' \,, \quad \text{where,}$$

$$[4] \quad g_j(x,x',y,y',z,z') = \frac{e^{-[\{y-y'\}/\sqrt{2}\,\sigma_y]^2}}{\sqrt{2u\pi}\cdot\sigma_y} \cdot \frac{e^{-[\{z-z'-v_j(x-x')/u\}/\sqrt{2}\,\sigma_z]^2}}{\sqrt{2u\pi}\cdot\sigma_z}$$

We place the detector at the origin of the system, temporarily. The spatial integral in y′ is taken to have infinite limits, but the x′ and z′ integrals are only integrated from 0 to some x_0 upwind and a maximum height h, respectively. We perform the integral over y′ which integrates to unity. The result is then:

$$[5] \qquad \langle c_j \rangle = \langle S_j \rangle \cdot \int_0^{x_0} \int_0^{h} \frac{e^{-[\{z'-v_j x'/u\}/\sqrt{2}\,\sigma_z]^2}}{\sqrt{2\pi}\cdot\sigma_z}\, dz'\, dx'$$

The z′ integral must be performed first, because the σ values depend on x′ in a power-law manner resulting in an integrand is not easily integrated in closed form. So we perform the z′ integral, obtaining,

$$[6] \qquad \langle c_j \rangle = \langle S_j \rangle \cdot \int_0^{x_0} \operatorname{erfc}(\phi_L(x')) - \operatorname{erfc}(\phi_U(x'))\, dx'$$

where $\phi_L(x') = \{0 - v_j\, x'/u\}/\sqrt{2}\,\sigma_Z$ and $\phi_U(x') = \{h - v_j\, x'/u\}/\sqrt{2}\,\sigma_Z$. This last integral, is performed numerically. After this is completed, the average source strength is completely determined from the assumed mean value of the detected concentration. Typically in this calculation, a value of h = 10 or 100 meters is used and x_0 is set in the range 1 to 10 km. It was found that for particle sizes of up to 35 μm, the settling velocity has a negligible effect on the value of the integral. As is discussed later, the two calculational parameters, x_0 and h, have an effect on the signal-to-noise ratio.

DETECTOR ARRAY

The code allows for a detector array of up to 25 detectors. By "detector" it is meant that there is a location where the particle count is determined and measured. No sort of detector hardware is simulated. We may then refer to these points as "perfect detectors." They are taken to have unit efficiency. No accounting is made for the statistics of particle collection. For instance, if the detector samples 1 cubic meter of air, with a mean particle count of 1/2 per cubic meter, the detector always registers 1/2 count.

Detectors should be centered near the origin of the coordinate system. When one specifies the "average concentration" for the purposes of normalization, it is taken to be that measured at the origin. A typical detector in the x-y plane (the plane of the ground) is shown in Fig. 2.

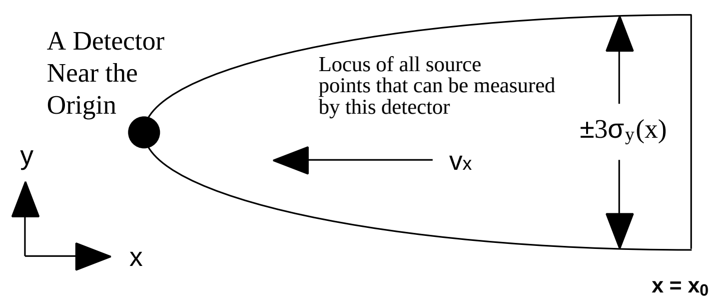

Figure 2. The locus of all source points in the x-y plane that can contribute to particle counts in a given detector. The width is determined by $\pm 3\,\sigma_y$,

In this drawing, the detector is the large black dot and the sources upwind that can contribute to the signal in the detector are contained within the closed contour (shown in the x-y plane). It is taken that the width of the contour is plus or minus three sigma. Although the model assumption is that there is a *uniform source infinitely distributed*, in fact there is no reason for the model to consider sources outside this contour because they cannot contribute to the signal.

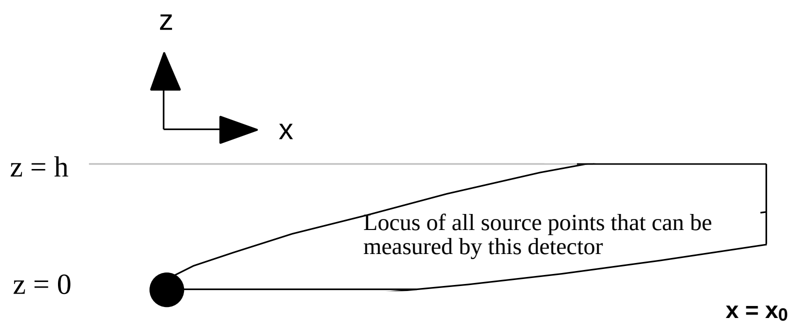

Figure 3. The locus of all source points in the x-z plane that can contribute to particle counts in a given detector. The width is determined by $\pm 3\ \sigma_z$, and also by the restriction that $0 < z < h$.

The situation in the x-z plane is different because of two reasons. One is that we have chosen that all sources shall be in the range $0 < z < h$. The other is that we must consider the particle settling. The result is that only the points within the closed contour in Fig. 3 can contribute to the counts in the detector. One interesting observation is that in the model for every non-zero particle settling velocity there is a value of x_0 for which the volume "pinches off". In other words, at some very large distance, the chances of a particle reaching the detector having originated at a height h becomes zero due to settling.

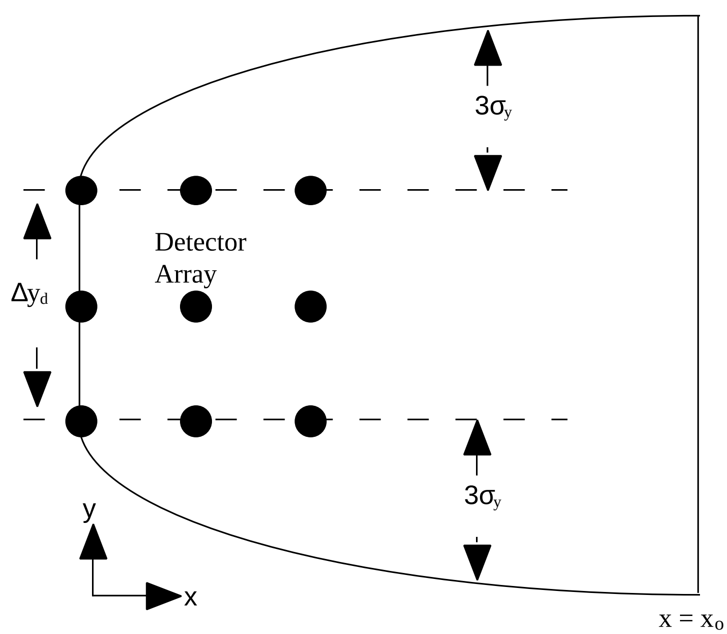

Figure 4. The locus of all source points in the x-y plane that can contribute to particle counts in any detector in an array of detectors. The width is determined by $\pm 3\ \sigma_y$, added to the width of the array.

Between these two drawings the reader can visualize the shape of the sampling volume for a single detector. Of course, one must first specify the location of each detector in an array before the sampling volume can be determined.

The case of an array versus a single detector increases the sampling volume because the union of all individual detector sampling volumes must be considered. The x-y view of the sampling volume of a 3x3 detector array is shown in Fig. 4 as an example.

HOW THE CODE WORKS

The user specifies through the input files the value of x_o and h. Once the detector array location has been determined through the input files, the code determines the average source strength by performing the integral of Equation [6]. The user specifies a source density Φ in units of per cubic km per second. The code computes the volume of source space, according to the logic of Figures 2 - 4. Each particle bin has a different volume, V_j, because the settling velocity differs. The actual sampling volume used in the computation is V, which is taken as the largest of all the V_j. The source frequency is then $\nu = V\Phi$. The code begins stepping forward in time, using a time interval Δt. The mean number of sources in this time interval is $\mu = \nu\Delta t$. The actual number of new sources in any interval is taken as a sample from a Poisson distribution with mean value μ. The x, y, and z coordinates of a given source are restricted to the sampling volume by a rejection method.[6]

The count in a given detector at a given time t is then given by a straightforward application of Equation [2]. Mathematically, it is assumed that each source (of index k) described by the Dirac delta function in time and space, with a given strength. The x, y, and z coordinate and time for a source are ξ_k, ψ_k, ζ_k, and τ_k, respectively. The source strength in bin j is $Q_{j,k}$. There are K sources present at a given time. The net source term for a given particle size bin is then:

$$[7] \qquad S_j(x',y',z',t') = \sum_{k=1}^{K} Q_{j,k}\, \delta(x' - \xi_k)\, \delta(y' - \psi_k)\, \delta(z' - \zeta_k)\, \delta(t' - \tau_k)$$

In order to determine the measured count rate in a given detector located at (x,y,z), Equation [7] is substituted into equation [2] and integrated. The result is:

$$[8] \qquad c_j(x,y,z,t) = \sum_{k=1}^{K} Q_{j,k}\, G_j(x, \xi_k, y, \psi_k, z, \zeta_k, t- \tau_k)$$

It should be noted that all particle sizes are represented with every source. In other words, Every source generates particles of all sizes. This is based on the empirical observation from some Dugway data that fluctuations in counts in particle bins tend to follow one another. However, for every source k, a fluctuation is given in the ratio of numbers of particles. In particular, the strength in a bin is taken as a Gaussian distribution, with the standard deviation equal to 1/5 of the expectation.

As time progresses, all sources that have been produced are kept in a “bank” unless it is determined that they have drifted far enough in x or z so that they can no longer contribute to the count in any detector. Therefore the code has a bank of sources that is continually added-to and removed-from. Depending on the value of x_o and h chosen, the number of sources in the bank can range from a dozen to a few thousand. Presently, the bank is limited to 2000 sources, which has tended to limit the value of x_o to about 10 km.

HOW TO USE THE CODE

The code is written in Microsoft FORTRAN Powerstation , Profession Edition, Version 4 for a Windows computer. Some of the IMSL library routines are used in the code. In order to use the code, starting from the source code, one must purchase this product from Microsoft or be willing to modify the code for another FORTRAN environment. If running, for instance, on a UNIX workstation, one would need to obtain the IMSL library, which is proprietary. If one cannot do this, some subroutine calls such as Poisson and Gaussian random number generators will have to be written from scratch or obtained from another library.

Presuming one has a running copy of the code all one needs to do is run the code and the code will write its own input files for a sample problem. This sample input file was chosen to mimic some of the Dugway data found on the ACTD web site.

3.0000	a_{DEB}	print quantity: 0 none . . > 5 dangerous
2.5000	u	wind speed, m/s
50.0000	h	max height of sources, m
2000.0	x_o	max x value of sources, m
10.0000	Δt	time interval for measurements, sec
4.0000	t_{max}	Log maximum time, sec
15.00	Φ	Probability Density New Sources,/s/km3
.0250	$\langle c \rangle$	mean baseline value (/m3)
.00000	ε	convergence in integration

Table 1. Main input file (unit 1) for the code. Name is G4_data.dat

The first line of the code is the print control. A value of 0 here minimizes the printed output. The only printing is to unit 31 and to the screen. Only the summary information is printed. If a_{deb} = 1 the time-dependent particle count in detector #1 is printed to the screen in a crude tab-graph format. If a_{deb} =2 the total particle count in all detectors (not bin information) is printed to unit 32. If a_{deb} = 3 all bin information for up to 25 detectors is written out. There is one output file per detector. If a_{deb} = 4 a table of sources is printed to unit 34. This can be quite large, depending on how many temporal measurements there are. If a_{deb} = 5 all Green's functions appearing in [8] are printed out. This also can be very long. The print control is inclusive of lower numbers, e.g., if you use a value of 4 you get all printing associated with a_{deb} = 3, 2 and 1.

The other lines in the input file are more straightforward. The wind speed in m/s is given in the second line. The user should input a positive value. The maximum height for sources, h and the maximum x value, x_o are input in the next two lines. The default values are recommended, but one can vary the distribution of measured intensities somewhat by adjusting these values. In general, a larger value for these two gives a smoother signal (more of a DC component) whereas smaller values, especially for x_o, give more of an AC component.

The time interval for measurements is given next, followed by the Log (base 10) of the maximum time. In principal, one may want this code to run for very long periods of time, provided that a_{deb} is set to 0 or 1 only. Then a value of, say, t_{max} =10, for the maximum time would be 10 billion seconds, or for practical purposes, forever. If you are printing detector files, with a_{deb} = 2 or 3, you will add a line to each output file at every measurement. You therefore want to limit the max time so as to give a few thousand measurements at most.

The probability density, Φ, is that value which when multiplied by the source volume gives the source frequency. For the sample problem, the computed volume is about 0.010 km^3. When multiplied by the value of Φ = 15 /s/km^3, the net source frequency ν is 1 source per every few seconds.

The mean baseline count value is input next. It is the expected mean value of total counts in the first detector in the array. The very last input in the file is ε, which may be used in place of x_o to compute the integral of equation [6]. The procedure which computes the integral then returns the value of x_o needed to give an accuracy within ε, of the value of the integral assuming an infinite upper limit. It is recommended to set $\varepsilon = 0$ always because the accuracy of this method is in doubt.

```
6.0000
0.40000   1.00
1.50000   1.00
3.50000   1.00
7.00000   1.00
15.0000   1.00
30.0000   1.00
```

Table 2. Particle bin size information input file for the code. Name is Size.dat

The default bin information is input through the file shown in Table 2. The first line of the file is the number of bins. Each line that follows contains an entry for the representative particle size in μm, and the expected relative mass intensity expected in that bin. The default shown is that each bin contributes equally in terms of mass to the total, which is not out of line with some empirical observations. However, one should remember that *mass per particle* is inversely proportional the cube of the diameter, so there will be far more of the smaller particles under these conditions.

```
9.0000
    .0000        .0000       .0000
  100.0000       .0000       .0000
 -100.0000       .0000       .0000
    .0000       100.00       .0000
  100.0000      100.00       .0000
 -100.0000      100.00       .0000
    .0000      -100.00       .0000
  100.0000     -100.00       .0000
 -100.0000     -100.00       .0000
```

Table 3. Detector location information input file for the code. Name is Det.dat

The detector information is shown in Table 3. Here the first line of the file shows the number of detectors and the subsequent lines show the detector locations. In all cases here the detectors are on the ground, so that the third entry is always zero.

CODE RESULTS

Total Counts In A Detector

The example shown above results in several output files. The main (unit 31) output file describes the general calculation and the summary of the results for each detector. Since we have chosen a time interval for measurements of 10 seconds and a total time of 10,000 seconds, we can expect 1000 separate measurements to be made in the simulation. The unit 32 output file contains the total count information for all 9 detectors for all 1000 measurements. In addition, there are 9 data files generated, one for each detector, containing all bin information.

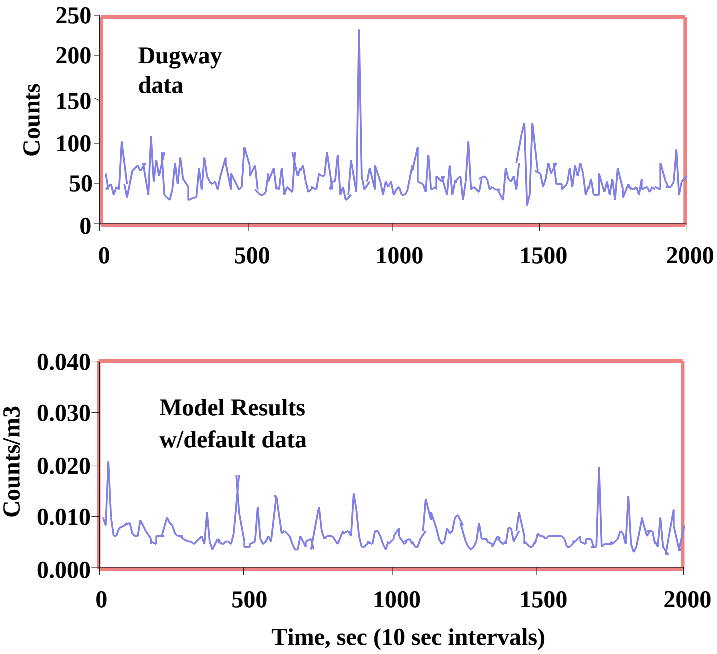

Figure 5. Comparison of code results with Dugway background data taken from the ACTD web site.

Total count results are shown in Figure 5 for the model, compared to data taken from the ACTD web site, Trial 1, Unit 2. The time interval for measurements is 10 seconds and the source frequency is apparently 10 seconds (however, higher actual source frequencies would not be observed because of the descretization of the data). The rise and fall times of the wiggles was found to be largely determined from the wind speed, which was measured to be 2.6 m/s during the test.

In the data and in the code results there is a DC component as well as a fluctuating component. The ratio of these two is adjusted by varying x_o. A value of 2 km for x_o was found to be good. Fine-tuning of the model may bring the results into closer agreement with the experimental data in the future. At this point it should be remembered that the model is only a model and can never be taken to truly represent reality.

Total Counts In Several Detectors

In Figure 6 the results from 3 of the 6 detectors is shown. The detectors are those along the y axis of the system, at three different x locations, as indicated. The farthest upwind detector's trace is on the top followed by the middle, followed by the detector most downwind. Some interesting results are seen immediately. The three peaks marked "A" are apparantly due to the same dust cloud passing through each of the detectors. Of course, the peak is both attenuated and shifted-in-time with distance downwind.

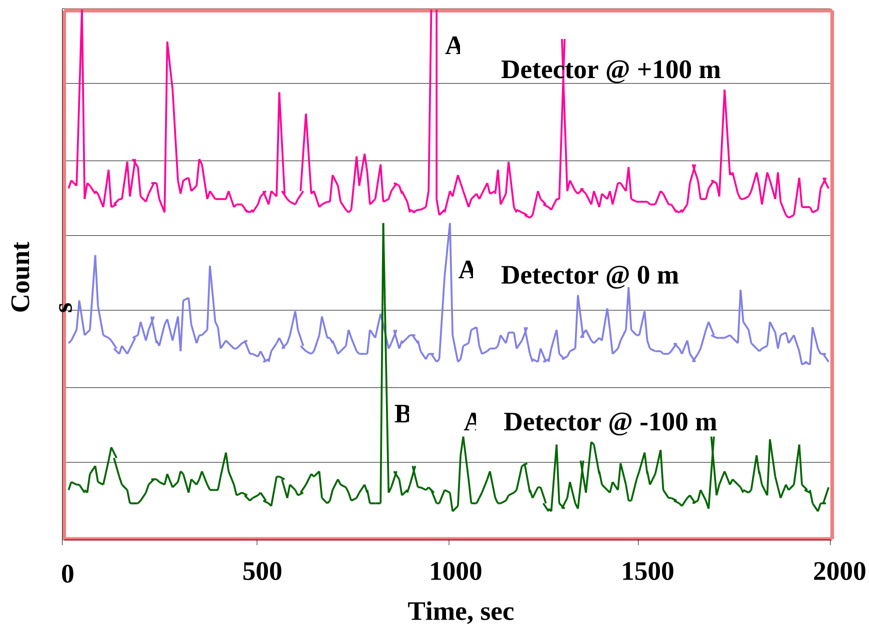

Figure 6. Total counts in three detectors in the array versus time. The spikes marked "A" are apparantly due to the same cloud passing through each detector. The spike "B" must have its source location physically between the second and third detector.

Particle Bin Counts

As was mentioned above, the code includes multi-bin capability based on particle size. The default input is equal intensity for all bins on a mass basis. When converted to particle counts, there are far more of the smallest particles compared to the larger ones. Figure 7 shows the results at one of the detectors in the array for the six different size bins. Fluctuations tend to follow one another in the model (but not exactly). If fluctuations were to follow one another, bin ratio values would be constant. In Figure 8 the ratio of the counts in the two smallest particle size bins is shown. There is jitter in this ratio.

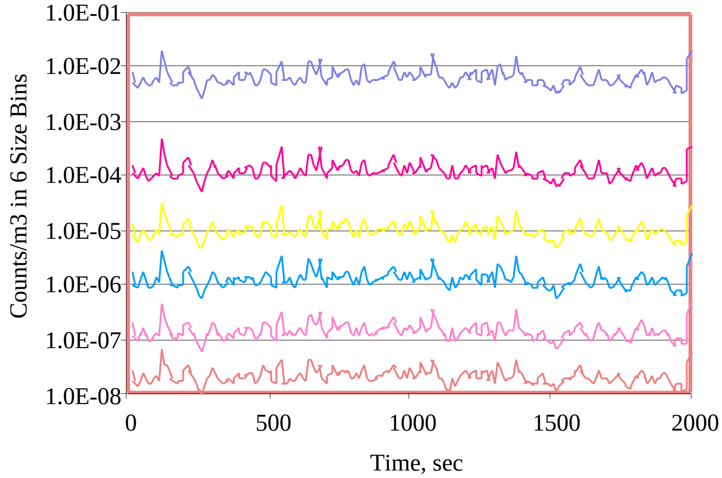

Figure 7. The six different particle size bins in one of the detectors in the array.

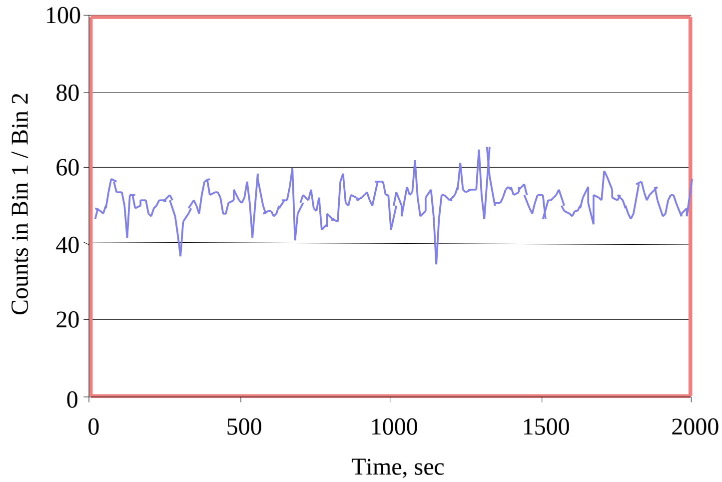

Figure 8. Ratio of counts in two of the bins in the previous figure.

ANOTHER LOOK AT THE DUGWAY DATA

The data taken from the ACTD web site was studied as to whether bin count ratio information may be more useful than simply total counts or counts in a given bin. It is to be remembered that the data contains both background and simulant release data. In all cases, the researchers release propylene gas into the air at the same time the simulant is released. There is a mass spectrometer co-located with the detectors which is able to detect the gas arrival accurately. It is therefore known exactly when the simulant has reached the detector, if one makes the reasonable assumption that the atmospheric transport of the gas and the simulant are similar .

Bin results are plotted in Figure 9. This is the same set of data as was shown in Figure 5, except with bin information. The APS counts in the raw data are separated into 62 bins.

To simplify the plots, these 62 bins were summed into 6 bins for the plot. It can be seen that the fluctuations in the bin counts do indeed follow one another in general.

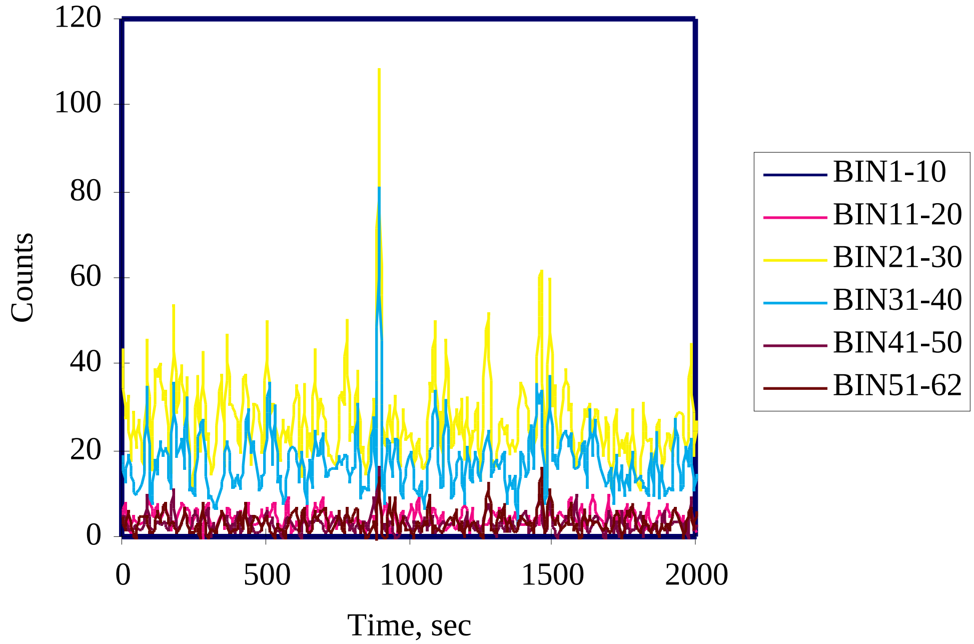

Figure 9. Counts in the APS counter at Dugway (62 bins) re-binned into 6 bins. It is seen that the count ratios do follow one another from bin-to bin.

Bin 41-50 counts are replotted in the upper half of Figure 10. The particle size range represented here is 7.23 μm to 13.8 μm. Also indicated is the cloud arrival time as determined by propylene data. The large spike to the left of the arrival is assumed to be a background fluctuation. It is doubted that any of the bin data by itself can be used to find the cloud arrival time. In the lower half of this Figure, however, is a plot of the *ratio* of counts in bins 41-50 to those in 21-30. The size range of bins 21-30 is 1.72 μm to 3.28 μm. It is seen that the background spike disappears and the true cloud arrival can be observed plainly.

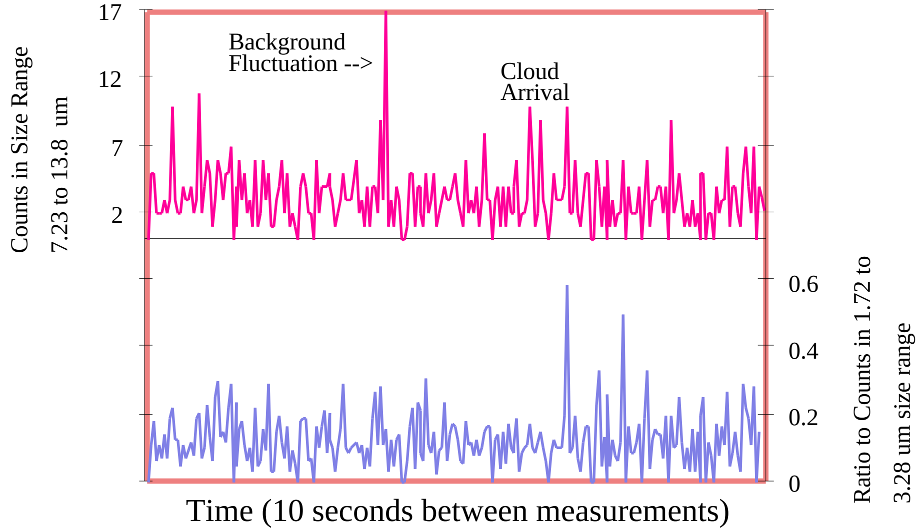

Figure 10. Dugway data plotted again, this time the upper half shows Bins 41-50 and the lower half shows the ratio to the counts in Bins 21-30. The true cloud arrival can be distinguished from the background by this manipulation of the data.

It is clear that much more insight can be derived by a study of the Dugway data located on the ACTD web site. Other sources of data will most certainly be required, though, because there is great variation in the behavior of the background worldwide and we do not believe that the Dugway Proving ground is representative of an average behavior for the world.

TO OBTAIN THE CODE

The code can be sent by email to any organization participating in the JBREWS program. Simply write or email the author (sailor@lanl.gov).

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[1] ACTD Web site is located at http://tig.sentel.com/actd.htm. Contact: Dr. David Cullin <dcullin@nswc.navy.mil>.

2. E. W. Peterson and B. Lighthart , Estimation Of Downwind Viable Airborne Microbes From A Wet Cooling-Tower : Including Settling *Microbial Ecology* V. 4(#1) Pp. 67-79 1977.

3. B. Lighthart and A. J. Mohr, editors, in "Atmospheric Microbial Aerosols, Theory and Applications”, Chapman and Hall, New York, 1994, pg 288.

[4] J. E. Till and H. R. Myers, eds., “Radiological Assessment: A Textbook on Environmental Dose Analysis”, Nuclear Regulatory Commission report NUREG/CR-3332, September 1983.

[5] National Oceanic and Atmospheric Administration report, “Report of the Meteorology Work Group, Southwest Energy Study - Appendix E”, US Department of Commerce, pg. 42, March 1972.

[6] Knuth, D. E., “The Art of Computing”, Vol. 2, “Seminumerical Algorithms”, Addison-Wesley Publishing Co., Reading, MA, 1969.